

Electronic Supplementary Material

Electronic Structure and Properties of Some Oligomers Based on Fluorinated 1*H*-Phospholes: *n*- vs. *p*-type Materials.

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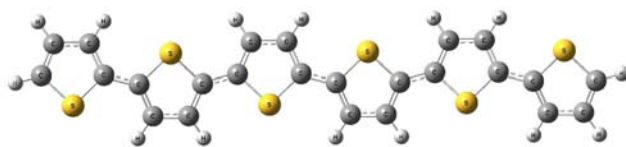
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Table 1S: Total energies of neutral (E), cation (E+) and anion (E-) form of Oligomers at B3LYP/SVP. Energy values are given in au.

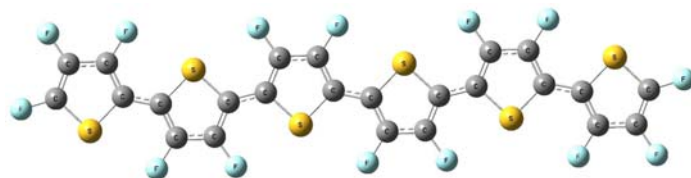
| Structures | E | E+ | E- |
|--------------------|----------------|----------------|----------------|
| 6T | -90064.11906 | -90058.293429 | -90065.407668 |
| PF-6T | -127825.365228 | -127818.949632 | -127827.255235 |
| FTTTTF | -3660.888215 | -3660.655863 | -3660.952194 |
| TFTTFT | -94189.319040 | -94182.936601 | -94190.902936 |
| 6-1 <i>H</i> -P | -80881.846478 | -80876.264694 | -80883.805225 |
| 6-1 <i>F</i> -P | -97069.84028 | -97063.92675 | -97072.63128 |
| PF-6P | -134832.955097 | -134826.461311 | -134835.998905 |
| 1 <i>H</i> -FPPPPF | -3435.942742 | -3435.717139 | -3436.025461 |
| 1 <i>H</i> -PFPPFP | -3832.65211 | -3832.418021 | -3832.758722 |
| 1 <i>F</i> -FPPPPF | -88067.85982 | -88061.62243 | -88069.81276 |
| 1 <i>F</i> -PFPPFP | -98859.63971 | -98853.16937 | -98862.16104 |

X, Y, Z coordinates at B3LYP/SVP.



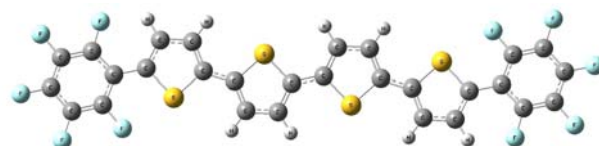
1. 6T

| | | | |
|---|----------|---------|---------|
| C | 11.0537 | 0.1256 | -0.1081 |
| C | 10.5335 | 1.3962 | -0.0750 |
| C | 9.1098 | 1.4065 | -0.0402 |
| C | 8.5487 | 0.1401 | -0.0469 |
| S | 9.8098 | -1.0767 | -0.0973 |
| C | 7.1497 | -0.2386 | -0.0199 |
| S | 5.8930 | 0.9817 | 0.0122 |
| C | 4.6195 | -0.2236 | 0.0338 |
| C | 5.1693 | -1.4961 | 0.0155 |
| C | 6.5854 | -1.5038 | -0.0157 |
| C | 3.2289 | 0.1698 | 0.0647 |
| S | 1.9545 | -1.0331 | 0.0162 |
| C | 0.6978 | 0.1872 | 0.0921 |
| C | 1.2651 | 1.4519 | 0.1437 |
| C | 2.6804 | 1.4421 | 0.1283 |
| C | -0.6978 | -0.1872 | 0.0921 |
| S | -1.9545 | 1.0331 | 0.0162 |
| C | -3.2289 | -0.1698 | 0.0647 |
| C | -2.6804 | -1.4421 | 0.1283 |
| C | -1.2651 | -1.4519 | 0.1437 |
| C | -4.6195 | 0.2236 | 0.0338 |
| C | -5.1693 | 1.4961 | 0.0155 |
| C | -6.5854 | 1.5038 | -0.0157 |
| C | -7.1497 | 0.2386 | -0.0199 |
| S | -5.8930 | -0.9817 | 0.0122 |
| H | -0.6694 | -2.3665 | 0.1993 |
| H | 0.6694 | 2.3665 | 0.1993 |
| H | -3.2897 | -2.3484 | 0.1683 |
| H | 3.2897 | 2.3484 | 0.1683 |
| H | -4.5620 | 2.4046 | 0.0262 |
| H | 4.5620 | -2.4046 | 0.0262 |
| H | -7.1825 | 2.4190 | -0.0321 |
| H | 7.1825 | -2.4190 | -0.0321 |
| H | 12.1013 | -0.1768 | -0.1383 |
| H | 11.1488 | 2.2994 | -0.0755 |
| H | 8.5111 | 2.3206 | -0.0105 |
| C | -8.5487 | -0.1401 | -0.0469 |
| C | -9.1098 | -1.4065 | -0.0402 |
| C | -10.5335 | -1.3962 | -0.0750 |
| S | -9.8098 | 1.0767 | -0.0973 |
| C | -11.0537 | -0.1256 | -0.1081 |
| H | -8.5111 | -2.3206 | -0.0105 |
| H | -11.1488 | -2.2994 | -0.0755 |
| H | -12.1013 | 0.1768 | -0.1383 |



2. PF-6T

| | | | | |
|----|---|----------|---------|--------|
| 1 | C | -11.0836 | -0.1684 | 0.0000 |
| 2 | C | -10.6144 | 1.1165 | 0.0000 |
| 3 | C | -9.1898 | 1.1478 | 0.0000 |
| 4 | C | -8.5829 | -0.0896 | 0.0000 |
| 5 | S | -9.8120 | -1.3582 | 0.0000 |
| 6 | C | -7.1719 | -0.3888 | 0.0000 |
| 7 | C | -6.5715 | -1.6320 | 0.0000 |
| 8 | C | -5.1585 | -1.5908 | 0.0000 |
| 9 | C | -4.6319 | -0.3133 | 0.0000 |
| 10 | S | -5.9396 | 0.8629 | 0.0000 |
| 11 | C | -3.2444 | 0.0704 | 0.0000 |
| 12 | S | -1.9372 | -1.1047 | 0.0000 |
| 13 | C | -0.7040 | 0.1484 | 0.0000 |
| 14 | C | -1.3069 | 1.3926 | 0.0000 |
| 15 | C | -2.7188 | 1.3491 | 0.0000 |
| 16 | C | 0.7040 | -0.1484 | 0.0000 |
| 17 | S | 1.9372 | 1.1047 | 0.0000 |
| 18 | C | 3.2444 | -0.0704 | 0.0000 |
| 19 | C | 2.7188 | -1.3491 | 0.0000 |
| 20 | C | 1.3069 | -1.3926 | 0.0000 |
| 21 | C | 4.6319 | 0.3133 | 0.0000 |
| 22 | S | 5.9396 | -0.8629 | 0.0000 |
| 23 | C | 7.1719 | 0.3888 | 0.0000 |
| 24 | C | 6.5715 | 1.6320 | 0.0000 |
| 25 | C | 5.1585 | 1.5908 | 0.0000 |
| 26 | C | 8.5829 | 0.0896 | 0.0000 |
| 27 | C | 9.1898 | -1.1478 | 0.0000 |
| 28 | C | 10.6144 | -1.1165 | 0.0000 |
| 29 | C | 11.0836 | 0.1684 | 0.0000 |
| 30 | S | 9.8120 | 1.3582 | 0.0000 |
| 31 | F | -12.3489 | -0.5487 | 0.0000 |
| 32 | F | -11.3655 | 2.2100 | 0.0000 |
| 33 | F | -8.5150 | 2.2956 | 0.0000 |
| 34 | F | -7.2522 | -2.7791 | 0.0000 |
| 35 | F | -4.4153 | -2.6963 | 0.0000 |
| 36 | F | -3.4645 | 2.4531 | 0.0000 |
| 37 | F | -0.6295 | 2.5400 | 0.0000 |
| 38 | F | 0.6295 | -2.5400 | 0.0000 |
| 39 | F | 3.4645 | -2.4531 | 0.0000 |
| 40 | F | 4.4153 | 2.6963 | 0.0000 |
| 41 | F | 7.2522 | 2.7791 | 0.0000 |
| 42 | F | 8.5150 | -2.2956 | 0.0000 |
| 43 | F | 11.3655 | -2.2100 | 0.0000 |
| 44 | F | 12.3489 | 0.5487 | 0.0000 |



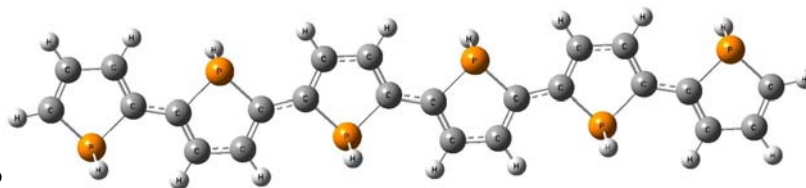
3. FTTFTF

| | | | | |
|----|---|----------|---------|---------|
| 1 | C | -7.1299 | 0.4809 | -0.1877 |
| 2 | C | -6.5110 | 1.6795 | -0.5157 |
| 3 | C | -5.0999 | 1.6158 | -0.5021 |
| 4 | C | -4.6047 | 0.3681 | -0.1565 |
| 5 | S | -5.9144 | -0.7437 | 0.1437 |
| 6 | C | -3.2284 | -0.0630 | -0.0445 |
| 7 | C | -2.7275 | -1.3287 | 0.2170 |
| 8 | C | -1.3150 | -1.3838 | 0.2531 |
| 9 | C | -0.7042 | -0.1607 | 0.0201 |
| 10 | S | -1.9142 | 1.0774 | -0.2448 |
| 11 | C | 0.7042 | 0.1607 | -0.0201 |
| 12 | S | 1.9142 | -1.0774 | 0.2448 |
| 13 | C | 3.2284 | 0.0630 | 0.0445 |
| 14 | C | 2.7275 | 1.3287 | -0.2170 |
| 15 | C | 1.3150 | 1.3838 | -0.2531 |
| 16 | C | 4.6047 | -0.3681 | 0.1565 |
| 17 | S | 5.9144 | 0.7437 | -0.1437 |
| 18 | C | 7.1299 | -0.4809 | 0.1877 |
| 19 | C | 6.5110 | -1.6795 | 0.5157 |
| 20 | C | 5.0999 | -1.6158 | 0.5021 |
| 21 | C | 8.5652 | -0.2019 | 0.0830 |
| 22 | H | 3.3682 | 2.1978 | -0.3737 |
| 23 | H | 4.4592 | -2.4640 | 0.7477 |
| 24 | H | 0.7530 | 2.2995 | -0.4432 |
| 25 | H | 7.0616 | -2.5820 | 0.7684 |
| 26 | H | -0.7530 | -2.2995 | 0.4432 |
| 27 | H | -3.3682 | -2.1978 | 0.3737 |
| 28 | H | -4.4592 | 2.4640 | -0.7477 |
| 29 | H | -7.0616 | 2.5820 | -0.7684 |
| 30 | C | -8.5652 | 0.2019 | -0.0830 |
| 31 | C | 9.5252 | -1.2345 | -0.0149 |
| 32 | C | 10.8945 | -0.9847 | -0.1041 |
| 33 | C | 11.3689 | 0.3284 | -0.1110 |
| 34 | C | 10.4552 | 1.3796 | -0.0252 |
| 35 | C | 9.0907 | 1.1082 | 0.0707 |
| 36 | F | 9.1499 | -2.5159 | -0.0320 |
| 37 | F | 11.7503 | -1.9976 | -0.1936 |
| 38 | F | 12.6699 | 0.5723 | -0.1992 |
| 39 | F | 10.8856 | 2.6368 | -0.0295 |
| 40 | F | 8.2693 | 2.1585 | 0.1505 |
| 41 | C | -9.0907 | -1.1082 | -0.0707 |
| 42 | C | -10.4552 | -1.3796 | 0.0252 |
| 43 | C | -11.3689 | -0.3284 | 0.1110 |
| 44 | C | -10.8945 | 0.9847 | 0.1041 |
| 45 | C | -9.5252 | 1.2345 | 0.0149 |
| 46 | F | -8.2693 | -2.1585 | -0.1505 |
| 47 | F | -10.8856 | -2.6368 | 0.0295 |
| 48 | F | -12.6699 | -0.5723 | 0.1992 |
| 49 | F | -11.7503 | 1.9976 | 0.1936 |
| 50 | F | -9.1499 | 2.5159 | 0.0320 |



4. TFFTFT

| | | | |
|---|---------|---------|----------|
| S | -0.8223 | 0.0604 | 2.0454 |
| S | 0.9713 | -0.0544 | 10.1415 |
| F | 2.6215 | 0.0499 | 5.1708 |
| F | 2.2256 | 0.0496 | 7.7273 |
| F | -2.4749 | -0.0190 | 7.0116 |
| F | -2.0792 | -0.0195 | 4.4548 |
| C | 0.2541 | -0.0152 | 0.6756 |
| C | 1.5724 | -0.0907 | 1.0997 |
| H | 2.4195 | -0.1518 | 0.4122 |
| C | 1.7153 | -0.0884 | 2.5046 |
| H | 2.6818 | -0.1464 | 3.0000 |
| C | 0.5087 | -0.0117 | 3.1938 |
| C | 0.2910 | 0.0091 | 4.6399 |
| C | 1.3474 | 0.0299 | 5.5766 |
| C | 1.1357 | 0.0329 | 6.9515 |
| C | -0.1446 | 0.0152 | 7.5433 |
| C | -1.2007 | 0.0025 | 6.6069 |
| C | -0.9896 | -0.0025 | 5.2318 |
| C | -0.3615 | 0.0114 | 8.9926 |
| C | -1.5681 | 0.0474 | 9.6821 |
| H | -2.5362 | 0.0927 | 9.1881 |
| C | -1.4192 | 0.0208 | 11.0945 |
| H | -2.2599 | 0.0435 | 11.7919 |
| C | -0.1032 | -0.0357 | 11.4854 |
| H | 0.2982 | -0.0653 | 12.4996 |
| S | 0.8151 | -0.0205 | -2.0447 |
| S | -0.9614 | 0.0421 | -10.1444 |
| F | -2.6249 | -0.0370 | -5.1780 |
| F | -2.2219 | -0.0393 | -7.7332 |
| F | 2.4766 | 0.0252 | -7.0044 |
| F | 2.0741 | 0.0248 | -4.4496 |
| C | -0.2647 | -0.0019 | -0.6759 |
| C | -1.5846 | 0.0239 | -1.1010 |
| H | -2.4343 | 0.0384 | -0.4141 |
| C | -1.7260 | 0.0262 | -2.5060 |
| H | -2.6938 | 0.0444 | -3.0019 |
| C | -0.5167 | 0.0017 | -3.1946 |
| C | -0.2959 | -0.0057 | -4.6402 |
| C | -1.3497 | -0.0205 | -5.5800 |
| C | -1.1342 | -0.0244 | -6.9544 |
| C | 0.1477 | -0.0082 | -7.5429 |
| C | 1.2011 | 0.0049 | -6.6035 |
| C | 0.9862 | 0.0089 | -5.2291 |
| C | 0.3687 | -0.0073 | -8.9914 |
| C | 1.5775 | -0.0373 | -9.6775 |
| H | 2.5445 | -0.0719 | -9.1806 |
| C | 1.4323 | -0.0197 | -11.0903 |
| H | 2.2752 | -0.0393 | -11.7853 |
| C | 0.1171 | 0.0239 | -11.4852 |
| H | -0.2818 | 0.0448 | -12.5007 |



5. 6-1H-P

| | | | | |
|----|---|---------|---------|----------|
| 1 | C | 0.1137 | 0.0482 | -11.3877 |
| 2 | P | -1.1659 | -0.0796 | -10.1040 |
| 3 | C | 0.1256 | 0.0033 | -8.7858 |
| 4 | C | -0.1543 | 0.0153 | -7.3706 |
| 5 | C | -1.3954 | 0.0510 | -6.7725 |
| 6 | C | -1.3945 | 0.0490 | -5.3375 |
| 7 | C | -0.1500 | 0.0117 | -4.7419 |
| 8 | C | 0.1324 | -0.0050 | -3.3335 |
| 9 | C | 1.3782 | -0.0403 | -2.7379 |
| 10 | C | 1.3814 | -0.0415 | -1.3056 |
| 11 | C | 0.1379 | -0.0069 | -0.7043 |
| 12 | C | -0.1379 | 0.0069 | 0.7043 |
| 13 | C | -1.3814 | 0.0415 | 1.3056 |
| 14 | C | -1.3782 | 0.0403 | 2.7379 |
| 15 | C | -0.1324 | 0.0050 | 3.3335 |
| 16 | C | 0.1500 | -0.0117 | 4.7419 |
| 17 | P | -1.1402 | -0.1330 | 6.0595 |
| 18 | C | 0.1543 | -0.0153 | 7.3706 |
| 19 | C | 1.3954 | -0.0510 | 6.7725 |
| 20 | C | 1.3945 | -0.0490 | 5.3375 |
| 21 | C | 1.3531 | -0.0458 | -10.8306 |
| 22 | C | 1.3641 | -0.0651 | -9.3818 |
| 23 | P | 1.1402 | 0.1330 | -6.0595 |
| 24 | P | -1.1581 | -0.1242 | -2.0165 |
| 25 | P | 1.1581 | 0.1242 | 2.0165 |
| 26 | H | 1.5731 | -1.2326 | -6.0624 |
| 27 | H | -2.3302 | 0.0708 | -7.3444 |
| 28 | H | -2.3279 | 0.0693 | -4.7634 |
| 29 | H | -1.5873 | 1.2426 | -2.0147 |
| 30 | H | 2.3106 | -0.0597 | -3.3135 |
| 31 | H | 2.3164 | -0.0619 | -0.7342 |
| 32 | H | -1.6312 | 1.2749 | -10.0680 |
| 33 | H | 2.2989 | -0.1258 | -8.8130 |
| 34 | H | 2.2784 | -0.1046 | -11.4146 |
| 35 | H | -0.0910 | 0.0603 | -12.4614 |
| 36 | H | 1.5873 | -1.2426 | 2.0147 |
| 37 | H | -2.3106 | 0.0597 | 3.3135 |
| 38 | H | -2.3164 | 0.0619 | 0.7342 |
| 39 | H | -1.5731 | 1.2326 | 6.0624 |
| 40 | H | 2.3279 | -0.0693 | 4.7634 |
| 41 | H | 2.3302 | -0.0708 | 7.3444 |
| 42 | C | -1.3641 | 0.0651 | 9.3818 |
| 43 | C | -1.3531 | 0.0458 | 10.8306 |
| 44 | C | -0.1256 | -0.0033 | 8.7858 |
| 45 | C | -0.1137 | -0.0482 | 11.3877 |
| 46 | P | 1.1659 | 0.0796 | 10.1040 |
| 47 | H | 1.6312 | -1.2749 | 10.0680 |
| 48 | H | -2.2989 | 0.1258 | 8.8130 |
| 49 | H | -2.2784 | 0.1046 | 11.4146 |
| 50 | H | 0.0910 | -0.0603 | 12.4614 |



6. 6-1F-P

| | | | | |
|----|---|----------|---------|---------|
| 1 | C | -7.3571 | -0.4267 | -0.0724 |
| 2 | C | -6.7110 | -1.6353 | -0.2210 |
| 3 | C | -5.2777 | -1.5788 | -0.2101 |
| 4 | C | -4.7326 | -0.3249 | -0.0377 |
| 5 | P | -6.0925 | 0.8659 | 0.2952 |
| 6 | C | -3.3329 | 0.0077 | 0.0008 |
| 7 | P | -1.9712 | -1.1923 | -0.3350 |
| 8 | C | -0.7096 | 0.1108 | 0.0127 |
| 9 | C | -1.3549 | 1.3184 | 0.1870 |
| 10 | C | -2.7862 | 1.2613 | 0.1809 |
| 11 | C | 0.7096 | -0.1108 | -0.0127 |
| 12 | P | 1.9712 | 1.1923 | 0.3350 |
| 13 | C | 3.3329 | -0.0077 | -0.0008 |
| 14 | C | 4.7326 | 0.3249 | 0.0377 |
| 15 | P | 6.0925 | -0.8659 | -0.2952 |
| 16 | C | 7.3571 | 0.4267 | 0.0724 |
| 17 | C | 6.7110 | 1.6353 | 0.2210 |
| 18 | C | 5.2777 | 1.5788 | 0.2101 |
| 19 | C | 2.7862 | -1.2613 | -0.1809 |
| 20 | C | 1.3549 | -1.3184 | -0.1870 |
| 21 | H | -1.9504 | -1.8578 | 0.9290 |
| 22 | H | -3.3943 | 2.1603 | 0.3195 |
| 23 | H | -0.8198 | 2.2620 | 0.3293 |
| 24 | H | 1.9504 | 1.8578 | -0.9290 |
| 25 | H | 0.8198 | -2.2620 | -0.3293 |
| 26 | H | 3.3943 | -2.1603 | -0.3195 |
| 27 | H | -6.0759 | 1.5882 | -0.9325 |
| 28 | H | -4.6740 | -2.4822 | -0.3366 |
| 29 | H | -7.2333 | -2.5829 | -0.3428 |
| 30 | C | -8.8036 | -0.2016 | -0.0394 |
| 31 | H | 6.0759 | -1.5882 | 0.9325 |
| 32 | C | 8.8036 | 0.2016 | 0.0394 |
| 33 | H | 7.2333 | 2.5829 | 0.3428 |
| 34 | H | 4.6740 | 2.4822 | 0.3366 |
| 35 | C | -9.7590 | -1.2405 | 0.0533 |
| 36 | C | -11.1331 | -1.0034 | 0.0749 |
| 37 | C | -11.6213 | 0.3035 | 0.0084 |
| 38 | C | -10.7163 | 1.3625 | -0.0785 |
| 39 | C | -9.3478 | 1.0999 | -0.1060 |
| 40 | F | -9.3744 | -2.5171 | 0.1375 |
| 41 | F | -11.9832 | -2.0215 | 0.1664 |
| 42 | F | -12.9277 | 0.5341 | 0.0295 |
| 43 | F | -11.1600 | 2.6136 | -0.1460 |
| 44 | F | -8.5302 | 2.1550 | -0.2013 |
| 45 | C | 9.3478 | -1.0999 | 0.1060 |
| 46 | C | 10.7163 | -1.3625 | 0.0785 |
| 47 | C | 11.6213 | -0.3035 | -0.0084 |
| 48 | C | 11.1331 | 1.0034 | -0.0749 |
| 49 | C | 9.7590 | 1.2405 | -0.0533 |
| 50 | F | 8.5302 | -2.1550 | 0.2013 |
| 51 | F | 11.1600 | -2.6136 | 0.1460 |
| 52 | F | 12.9277 | -0.5341 | -0.0295 |
| 53 | F | 11.9832 | 2.0215 | -0.1664 |
| 54 | F | 9.3744 | 2.5171 | -0.1375 |



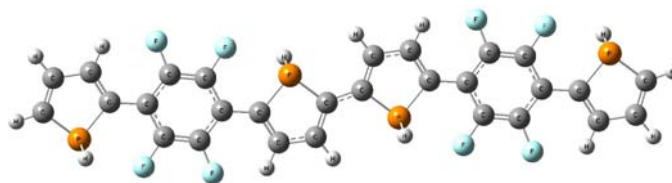
7. PF-6P

| | | | | |
|----|---|----------|---------|---------|
| 1 | P | -10.3352 | -1.0341 | -0.2622 |
| 2 | C | -11.7145 | 0.1005 | 0.0172 |
| 3 | C | -11.2620 | 1.3833 | 0.0817 |
| 4 | C | -9.8199 | 1.5139 | 0.0859 |
| 5 | C | -9.1228 | 0.3270 | 0.0270 |
| 6 | H | -10.2972 | -1.7342 | 0.9823 |
| 7 | H | -12.7679 | -0.1907 | -0.0115 |
| 8 | H | -11.9146 | 2.2621 | 0.1233 |
| 9 | H | -9.3428 | 2.4931 | 0.1311 |
| 10 | C | -7.6687 | 0.1595 | 0.0234 |
| 11 | C | -6.7441 | 1.2265 | -0.0155 |
| 12 | C | -5.3683 | 1.0263 | -0.0072 |
| 13 | C | -4.7620 | -0.2483 | 0.0375 |
| 14 | C | -5.6877 | -1.3155 | 0.0785 |
| 15 | C | -7.0633 | -1.1145 | 0.0703 |
| 16 | F | -7.1654 | 2.4946 | -0.0746 |
| 17 | F | -4.5948 | 2.1201 | -0.0593 |
| 18 | F | -5.2658 | -2.5836 | 0.1363 |
| 19 | F | -7.8370 | -2.2080 | 0.1181 |
| 20 | C | -3.3115 | -0.4159 | 0.0230 |
| 21 | P | -2.0989 | 0.9490 | 0.2929 |
| 22 | C | -0.6936 | -0.1978 | 0.0049 |
| 23 | C | -1.1837 | -1.4838 | -0.0697 |
| 24 | C | -2.6134 | -1.6051 | -0.0535 |
| 25 | H | -2.1391 | 1.5990 | -0.9784 |
| 26 | H | -0.5417 | -2.3686 | -0.1451 |
| 27 | H | -3.0938 | -2.5823 | -0.1036 |
| 28 | C | 0.6936 | 0.1978 | -0.0049 |
| 29 | C | 1.1837 | 1.4838 | 0.0697 |
| 30 | C | 2.6134 | 1.6051 | 0.0535 |
| 31 | C | 3.3115 | 0.4159 | -0.0230 |
| 32 | P | 2.0989 | -0.9490 | -0.2929 |
| 33 | H | 0.5417 | 2.3686 | 0.1451 |
| 34 | H | 3.0938 | 2.5823 | 0.1036 |
| 35 | H | 2.1391 | -1.5990 | 0.9784 |
| 36 | C | 4.7620 | 0.2483 | -0.0375 |
| 37 | C | 5.6877 | 1.3155 | -0.0785 |
| 38 | C | 7.0633 | 1.1145 | -0.0703 |
| 39 | C | 7.6687 | -0.1595 | -0.0234 |
| 40 | C | 6.7441 | -1.2265 | 0.0155 |
| 41 | C | 5.3683 | -1.0263 | 0.0072 |
| 42 | F | 5.2658 | 2.5836 | -0.1363 |
| 43 | F | 7.8370 | 2.2080 | -0.1181 |
| 44 | F | 7.1654 | -2.4946 | 0.0746 |
| 45 | F | 4.5948 | -2.1201 | 0.0593 |
| 46 | C | 9.1228 | -0.3270 | -0.0270 |
| 47 | P | 10.3352 | 1.0341 | 0.2622 |
| 48 | C | 11.7145 | -0.1005 | -0.0172 |
| 49 | C | 11.2620 | -1.3833 | -0.0817 |
| 50 | C | 9.8199 | -1.5139 | -0.0859 |
| 51 | H | 10.2972 | 1.7342 | -0.9823 |
| 52 | H | 12.7679 | 0.1907 | 0.0115 |
| 53 | H | 11.9146 | -2.2621 | -0.1233 |
| 54 | H | 9.3428 | -2.4931 | -0.1311 |



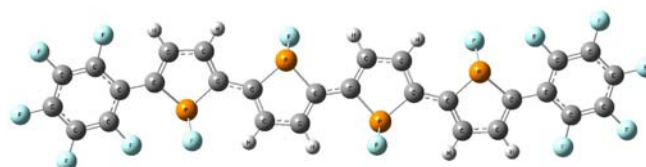
8. 1H-FPPPPF

| | | | | |
|----|---|---------|---------|----------|
| 1 | C | 0.2841 | 0.0426 | -11.3433 |
| 2 | C | 1.5057 | 0.2129 | -10.7710 |
| 3 | C | 1.5139 | 0.1873 | -9.3112 |
| 4 | C | 0.2849 | -0.0245 | -8.7396 |
| 5 | C | -0.0355 | -0.0321 | -7.3409 |
| 6 | P | 1.1210 | 0.5287 | -6.0150 |
| 7 | C | -0.0786 | -0.0180 | -4.7185 |
| 8 | C | 0.1984 | -0.0119 | -3.3174 |
| 9 | P | -1.0013 | -0.5595 | -2.0224 |
| 10 | C | 0.1595 | -0.0027 | -0.6954 |
| 11 | C | -0.1595 | 0.0027 | 0.6954 |
| 12 | P | 1.0013 | 0.5595 | 2.0224 |
| 13 | C | -0.1984 | 0.0119 | 3.3174 |
| 14 | C | 0.0786 | 0.0180 | 4.7185 |
| 15 | C | 1.2972 | 0.2318 | 5.3282 |
| 16 | C | 1.2715 | 0.2404 | 6.7705 |
| 17 | C | 0.0355 | 0.0321 | 7.3409 |
| 18 | C | -0.2849 | 0.0245 | 8.7396 |
| 19 | P | 0.8964 | 0.5173 | 10.0792 |
| 20 | C | -0.2841 | -0.0426 | 11.3433 |
| 21 | C | -1.5057 | -0.2129 | 10.7710 |
| 22 | C | -1.5139 | -0.1873 | 9.3112 |
| 23 | P | -0.8964 | -0.5173 | -10.0792 |
| 24 | C | -1.2715 | -0.2404 | -6.7705 |
| 25 | C | -1.2972 | -0.2318 | -5.3282 |
| 26 | C | 1.4190 | 0.2027 | -2.7083 |
| 27 | C | 1.3981 | 0.2075 | -1.2697 |
| 28 | C | -1.3981 | -0.2075 | 1.2697 |
| 29 | C | -1.4190 | -0.2027 | 2.7083 |
| 30 | P | -1.1210 | -0.5287 | 6.0150 |
| 31 | F | 2.2840 | -0.6280 | -5.9861 |
| 32 | H | -2.1821 | -0.4017 | -7.3577 |
| 33 | H | -2.2278 | -0.3855 | -4.7710 |
| 34 | F | -2.1586 | 0.6031 | -2.0428 |
| 35 | H | 2.3474 | 0.3593 | -3.2684 |
| 36 | H | 2.3097 | 0.3671 | -0.6837 |
| 37 | F | -2.0593 | 0.6323 | -9.9846 |
| 38 | H | 2.4358 | 0.3275 | -8.7365 |
| 39 | H | 2.4315 | 0.3475 | -11.3423 |
| 40 | H | 0.1023 | -0.0076 | -12.4201 |
| 41 | F | 2.1586 | -0.6031 | 2.0428 |
| 42 | H | -2.3474 | -0.3593 | 3.2684 |
| 43 | H | -2.3097 | -0.3671 | 0.6837 |
| 44 | F | -2.2840 | 0.6280 | 5.9861 |
| 45 | H | 2.2278 | 0.3855 | 4.7710 |
| 46 | H | 2.1821 | 0.4017 | 7.3577 |
| 47 | F | 2.0593 | -0.6323 | 9.9846 |
| 48 | H | -2.4358 | -0.3275 | 8.7365 |
| 49 | H | -2.4315 | -0.3475 | 11.3423 |
| 50 | H | -0.1023 | 0.0076 | 12.4201 |



9. 1F-FPPPPF

| | | | | |
|----|---|---------|---------|----------|
| 1 | C | -0.0338 | -0.1080 | -11.4222 |
| 2 | C | 1.2073 | 0.0104 | -10.9028 |
| 3 | C | 1.2127 | 0.0641 | -9.4402 |
| 4 | C | 0.0065 | -0.0370 | -8.8173 |
| 5 | C | -0.2427 | 0.0193 | -7.4058 |
| 6 | P | 1.0245 | 0.4278 | -6.1058 |
| 7 | C | -0.2045 | 0.0678 | -4.7561 |
| 8 | C | 0.0801 | 0.0619 | -3.3546 |
| 9 | P | -1.1478 | -0.3482 | -2.0172 |
| 10 | C | 0.1209 | 0.0130 | -0.7042 |
| 11 | C | -0.1209 | -0.0130 | 0.7042 |
| 12 | P | 1.1478 | 0.3482 | 2.0172 |
| 13 | C | -0.0801 | -0.0619 | 3.3546 |
| 14 | C | 0.2045 | -0.0678 | 4.7561 |
| 15 | C | 1.4342 | 0.0511 | 5.3389 |
| 16 | C | 1.4536 | 0.0801 | 6.7857 |
| 17 | C | 0.2427 | -0.0193 | 7.4058 |
| 18 | C | -0.0065 | 0.0370 | 8.8173 |
| 19 | P | 1.2818 | 0.4446 | 10.1026 |
| 20 | C | 0.0338 | 0.1080 | 11.4222 |
| 21 | C | -1.2073 | -0.0104 | 10.9028 |
| 22 | C | -1.2127 | -0.0641 | 9.4402 |
| 23 | P | -1.2818 | -0.4446 | -10.1026 |
| 24 | C | -1.4536 | -0.0801 | -6.7857 |
| 25 | C | -1.4342 | -0.0511 | -5.3389 |
| 26 | C | 1.3090 | 0.1817 | -2.7686 |
| 27 | C | 1.3313 | 0.1561 | -1.3237 |
| 28 | C | -1.3313 | -0.1561 | 1.3237 |
| 29 | C | -1.3090 | -0.1817 | 2.7686 |
| 30 | P | -1.0245 | -0.4278 | 6.1058 |
| 31 | F | 1.9226 | -0.9298 | -6.0968 |
| 32 | F | -2.0458 | 1.0090 | -1.9759 |
| 33 | F | -2.1707 | 0.9177 | -10.1253 |
| 34 | F | 2.0458 | -1.0090 | 1.9759 |
| 35 | F | -1.9226 | 0.9298 | 6.0968 |
| 36 | F | 2.1707 | -0.9177 | 10.1253 |
| 37 | F | 0.3119 | 0.2187 | 12.7146 |
| 38 | F | -2.3472 | -0.0571 | 11.5716 |
| 39 | F | -2.3792 | -0.2118 | 8.8241 |
| 40 | F | 2.6210 | 0.2092 | 7.4116 |
| 41 | F | 2.5829 | 0.1507 | 4.6781 |
| 42 | F | -2.4554 | -0.3152 | 3.4285 |
| 43 | F | -2.4972 | -0.2714 | 0.6958 |
| 44 | F | 2.4972 | 0.2714 | -0.6958 |
| 45 | F | 2.4554 | 0.3152 | -3.4285 |
| 46 | F | -2.5829 | -0.1507 | -4.6781 |
| 47 | F | -2.6210 | -0.2092 | -7.4116 |
| 48 | F | -0.3119 | -0.2187 | -12.7146 |
| 49 | F | 2.3472 | 0.0571 | -11.5716 |
| 50 | F | 2.3792 | 0.2118 | -8.8241 |



10. 1H-PFPPFP

| | | | | |
|----|---|----------|---------|---------|
| 1 | C | 9.7240 | -0.1336 | 1.3369 |
| 2 | C | 8.7754 | 0.0076 | 0.2964 |
| 3 | C | 9.3248 | 0.0665 | -1.0043 |
| 4 | C | 10.6936 | 0.0107 | -1.2610 |
| 5 | C | 11.5905 | -0.1311 | -0.2010 |
| 6 | C | 11.0967 | -0.2010 | 1.1039 |
| 7 | C | 7.3303 | 0.0445 | 0.5165 |
| 8 | C | 6.6713 | 0.0632 | 1.7247 |
| 9 | C | 5.2290 | 0.0712 | 1.6577 |
| 10 | C | 4.7037 | 0.0668 | 0.3880 |
| 11 | P | 6.0747 | 0.4007 | -0.7954 |
| 12 | F | 8.5164 | 0.1947 | -2.0601 |
| 13 | F | 11.1439 | 0.0810 | -2.5084 |
| 14 | F | 12.8952 | -0.1930 | -0.4278 |
| 15 | F | 11.9394 | -0.3333 | 2.1227 |
| 16 | F | 9.3326 | -0.2094 | 2.6119 |
| 17 | C | 3.3212 | 0.0078 | 0.0215 |
| 18 | C | 2.7961 | 0.0013 | -1.2526 |
| 19 | C | 1.3576 | -0.0137 | -1.3267 |
| 20 | C | 0.7053 | -0.0196 | -0.1118 |
| 21 | P | 1.9542 | -0.3556 | 1.2079 |
| 22 | C | -0.7053 | 0.0196 | 0.1118 |
| 23 | C | -1.3576 | 0.0137 | 1.3267 |
| 24 | C | -2.7961 | -0.0013 | 1.2526 |
| 25 | C | -3.3212 | -0.0078 | -0.0215 |
| 26 | P | -1.9542 | 0.3556 | -1.2079 |
| 27 | C | -4.7037 | -0.0668 | -0.3880 |
| 28 | P | -6.0747 | -0.4007 | 0.7954 |
| 29 | C | -7.3303 | -0.0445 | -0.5165 |
| 30 | C | -8.7754 | -0.0076 | -0.2964 |
| 31 | C | -9.7240 | 0.1336 | -1.3369 |
| 32 | C | -11.0967 | 0.2010 | -1.1039 |
| 33 | C | -11.5905 | 0.1311 | 0.2010 |
| 34 | C | -10.6936 | -0.0107 | 1.2610 |
| 35 | C | -9.3248 | -0.0665 | 1.0043 |
| 36 | F | -9.3326 | 0.2094 | -2.6119 |
| 37 | F | -11.9394 | 0.3333 | -2.1227 |
| 38 | F | -12.8952 | 0.1930 | 0.4278 |
| 39 | F | -11.1439 | -0.0810 | 2.5084 |
| 40 | F | -8.5164 | -0.1947 | 2.0601 |
| 41 | C | -6.6713 | -0.0632 | -1.7247 |
| 42 | C | -5.2290 | -0.0712 | -1.6577 |
| 43 | F | -1.8885 | -0.9784 | -2.1587 |
| 44 | H | -3.4155 | -0.0064 | 2.1538 |
| 45 | H | -0.8340 | 0.0193 | 2.2870 |
| 46 | F | 1.8885 | 0.9784 | 2.1587 |
| 47 | H | 0.8340 | -0.0193 | -2.2870 |
| 48 | H | 3.4155 | 0.0064 | -2.1538 |
| 49 | F | -6.0260 | 0.9223 | 1.7540 |
| 50 | H | -4.6193 | -0.0803 | -2.5655 |
| 51 | H | -7.1802 | -0.0824 | -2.6872 |
| 52 | F | 6.0260 | -0.9223 | -1.7540 |
| 53 | H | 7.1802 | 0.0824 | 2.6872 |
| 54 | H | 4.6193 | 0.0803 | 2.5655 |



11. 1F-PFPPFP

| | | | | |
|----|---|----------|---------|---------|
| 1 | C | 5.3370 | 1.1019 | 0.1290 |
| 2 | C | 4.7577 | -0.1828 | 0.0262 |
| 3 | C | 5.6987 | -1.2244 | -0.1398 |
| 4 | C | 7.0694 | -0.9965 | -0.1848 |
| 5 | C | 7.6468 | 0.2882 | -0.0846 |
| 6 | C | 6.7070 | 1.3297 | 0.0829 |
| 7 | C | 3.3134 | -0.3798 | 0.0440 |
| 8 | P | 2.0773 | 0.9472 | 0.4154 |
| 9 | C | 0.6889 | -0.1990 | 0.0304 |
| 10 | C | 1.1888 | -1.4786 | 0.0086 |
| 11 | C | 2.6308 | -1.5764 | 0.0198 |
| 12 | F | 5.2930 | -2.4927 | -0.2572 |
| 13 | F | 7.8594 | -2.0650 | -0.3391 |
| 14 | C | 9.0925 | 0.4956 | -0.1063 |
| 15 | C | 9.7611 | 1.6919 | -0.1636 |
| 16 | C | 11.2176 | 1.5907 | -0.1130 |
| 17 | C | 11.6976 | 0.3265 | -0.0050 |
| 18 | P | 10.3531 | -0.8482 | -0.3232 |
| 19 | F | 7.1128 | 2.5976 | 0.2025 |
| 20 | F | 4.5460 | 2.1699 | 0.2872 |
| 21 | C | -0.6889 | 0.1990 | -0.0304 |
| 22 | C | -1.1888 | 1.4786 | -0.0086 |
| 23 | C | -2.6308 | 1.5764 | -0.0198 |
| 24 | C | -3.3134 | 0.3798 | -0.0440 |
| 25 | P | -2.0773 | -0.9472 | -0.4154 |
| 26 | C | -4.7577 | 0.1828 | -0.0262 |
| 27 | C | -5.3370 | -1.1019 | -0.1290 |
| 28 | C | -6.7070 | -1.3297 | -0.0829 |
| 29 | C | -7.6468 | -0.2882 | 0.0846 |
| 30 | C | -7.0694 | 0.9965 | 0.1848 |
| 31 | C | -5.6987 | 1.2244 | 0.1398 |
| 32 | C | -9.0925 | -0.4956 | 0.1063 |
| 33 | C | -9.7611 | -1.6919 | 0.1636 |
| 34 | C | -11.2176 | -1.5907 | 0.1130 |
| 35 | C | -11.6976 | -0.3265 | 0.0050 |
| 36 | P | -10.3531 | 0.8482 | 0.3232 |
| 37 | F | -7.1128 | -2.5976 | -0.2025 |
| 38 | F | -4.5460 | -2.1699 | -0.2872 |
| 39 | F | -5.2930 | 2.4927 | 0.2572 |
| 40 | F | -7.8594 | 2.0650 | 0.3391 |
| 41 | F | -10.2532 | 1.7499 | -1.0313 |
| 42 | H | -12.7567 | -0.0563 | -0.0162 |
| 43 | H | -11.8466 | -2.4860 | 0.1725 |
| 44 | H | -9.2716 | -2.6622 | 0.2565 |
| 45 | F | -2.0729 | -1.9356 | 0.8864 |
| 46 | H | -0.5610 | 2.3756 | 0.0171 |
| 47 | H | -3.1200 | 2.5512 | -0.0177 |
| 48 | H | 0.5610 | -2.3756 | -0.0171 |
| 49 | H | 3.1200 | -2.5512 | 0.0177 |
| 50 | F | 2.0729 | 1.9356 | -0.8864 |
| 51 | F | 10.2532 | -1.7499 | 1.0313 |
| 52 | H | 12.7567 | 0.0563 | 0.0162 |
| 53 | H | 11.8466 | 2.4860 | -0.1725 |
| 54 | H | 9.2716 | 2.6622 | -0.2565 |

Figure 1S. DFT//B3LYP/3-21G(d) Raman profiles (un-scaled, in cm^{-1}) of oligomers

